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NAVWEPS REPORT 7646

NOTS TP 2663

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## CALCULATION OF CRITICAL TEMPERATURE AND TIME-TO-EXPLOSION FOR PROPELLANTS AND EXPLOSIVES

By

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**ABSTRACT.** The solutions available in the literature for the critical temperature of various geometric shapes and boundary conditions are gathered together, and a nomograph is presented, which greatly facilitates numerical calculation of the critical temperature for specific cases.

Nomographs are also presented for the numerical calculation of the time required to cause explosion in the event the temperature at the surface of an object is held at a temperature greater than critical.

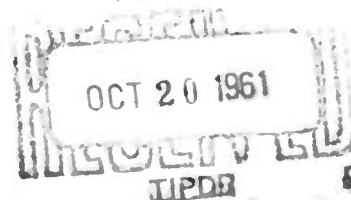
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U. S. NAVAL ORDNANCE TEST STATION

China Lake, California

March 1961



# U. S. NAVAL ORDNANCE TEST STATION

## AN ACTIVITY OF THE BUREAU OF NAVAL WEAPONS

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WM. B. McLEAN, PH.D.  
*Technical Director*

### FOREWORD

The Explosives and Pyrotechnics Division has been conducting research and development on explosives and supplying these new explosives, as they are needed for particular weapons, to the U. S. Naval Ordnance Test Station and elsewhere. The problems of aerodynamic heating of missiles and safety in case of fire prompted the Division to seek ways of predicting times-to-explosion at any temperature for any mass of explosive or propellant. The uses of data as evolved through adiabatic-autoignition determination are expressed in nomographs as an aid to those who need to know how long a given explosive warhead or complete missile assembly will be safe under expected temperature conditions.

This report was reviewed for technical accuracy by C. D. Lind of the Propulsion Development Department and R. G. S. Sewell of the Weapons Development Department.

This project was supported by Task Assignment RUUO-3E-015/216-1/F008-10-004.

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the authority of:

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Department*

NOTS Technical Publication 2663  
NAVWEPS Report 7646

Published by ..... Publishing Division  
Technical Information Department  
Collation ..... Cover, 9 leaves, abstract cards  
First printing ..... 175 numbered copies  
Security classification ..... UNCLASSIFIED

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## NOMENCLATURE

<i>a</i>	Exterior radius, half-thickness of slab, cm
<i>c</i>	Specific heat capacity, cal/g-°C
<i>d</i>	Differential operator
<i>E</i>	Activation energy, cal/mole (also in kcal/mole on nomographs)
<i>F</i>	Function $\lambda t_e / \rho c a^2$
<i>F( )</i>	One function of the quantity in parenthesis
<i>f( )</i>	One function of the quantity in parenthesis
<i>h</i>	Heat-transfer coefficient, cal/cm <sup>2</sup> -sec-°C
<i>k</i>	Parameter in Eq. 3
log	Logarithm to base 10
<i>M</i>	Modulus cm/unit of linearly plotted variable
<i>QZ</i>	Heat release parameter, cal/g-sec
<i>R</i>	Universal gas constant, 1.987 cal/mole-°K
<i>r</i>	Radius, distance from central plane of slab, cm
<i>T</i>	Temperature, °K
<i>T<sub>m</sub></i>	Critical temperature, °K
<i>T<sub>s</sub></i>	Temperature of surface of object, °K
<i>T<sub>0</sub></i>	Temperature of surroundings, °K
<i>T<sub>1</sub></i>	Constant temperature of surface, held at value greater than critical temperature, °K

$T^*$	$1/(1/T_m - 1/T_1)$ , °K
$t$	Time, sec
$t_e$	Time-to-explosion, sec
$x, y, z$	Variables in formulas for types of nomographs
$Z$	See QZ
$\alpha, \beta$	Axes on nomographs
$\delta$	Shape factor, Eq. 4. Numerical values herein are critical values of $\delta$ , see Eq. 9
$\theta$	Dimensionless variable $E(T - T_0)/RT_0^2$
$\theta_s$	Value of $\theta$ at surface
$\lambda$	Thermal conductivity, cal/cm-sec-°C
$\rho$	Density gm/cm <sup>3</sup>
$\phi( )$	One function of the quantity in parenthesis
$\psi( )$	One function of the quantity in parenthesis
$\omega$	Dimensionless distance, $r/a$
$\partial$	Partial differential operator
$\nabla^2$	Laplacian operator of vector analysis

### ACKNOWLEDGMENT

The included nomographs were made at the suggestion of Dr. Douglas Lind, Propulsion Development Department, who is making experimental measurements of the decomposition-rate parameters for various explosives and propellants. Dr. Lind was also of assistance in the selection of ranges for variables and nomenclature on the nomographs.

## INTRODUCTION

It has been known for some time that many materials, including propellants and high explosives, can exhibit the phenomenon of self-heating. This is the liberation of energy in the interior of the material caused by a slow chemical reaction that is often a decomposition reaction. If this heat is not removed from the material, the temperature of the material increases with a concurrent increase in the rate of reaction. If the material is not disturbed, a state of dynamic equilibrium will be reached at which heat is removed as fast as it is generated; or, if heat cannot be removed sufficiently fast, the temperature increases more and more rapidly, and eventually the material catches fire or explodes if it is capable of so doing.

The quantitative description of this type of situation has been relatively recent. The differential equation describing the situation is well known and may be written as

$$\rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + \rho Q Z \exp(-E/RT) \quad (1)$$

in which it is assumed that the thermal conductivity,  $\lambda$ , is independent of position and that the energy liberated by chemical reaction is given in terms of cal/cm<sup>3</sup>-sec by the expression  $\rho Q Z \exp(-E/RT)$ . This partial differential equation is strongly nonlinear and has not been solved until recently.

If a steady-state temperature distribution can be attained, it will satisfy the ordinary nonlinear differential equation

$$\lambda \nabla^2 T + \rho Q Z \exp(-E/RT) = 0 \quad (2)$$

Frank-Kamenetski (Ref. 1) obtained the steady-state solution for a slab with both faces held at a constant temperature; Chambré (Ref. 2) gave the steady-state solutions for the cylinder and the sphere with their outer surfaces held at a constant temperature; and Enig (Ref. 3) presented the steady-state solution for the hollow cylinder with its surfaces held at constant temperatures. Longwell and Conrad (Ref. 4) presented the solution for the hollow cylinder with its exterior surface held at a constant temperature and its interior surface adiabatic. The above solutions were all analytical and employ an approximation that represents the exponential of the reciprocal temperature as an exponential of a direct temperature function. Enig, Shanks, and Southworth (Ref. 5) made numerical solutions for the steady state, which did not use this approximation. Constant-temperature surfaces were taken for the slab, the cylinder, and the sphere, and their results agreed well with those found earlier for situations ordinarily encountered.

The foregoing authors all used constant-temperature surfaces. This implies relatively large heat-transfer coefficients. Thomas (Ref. 6) obtained solutions for the steady state for the slab, the cylinder, and the sphere as functions of the heat-transfer coefficients to the surroundings that were taken to be at constant temperature.

Gray and Harper (Ref. 7) assumed that the thermal conductivity was large in comparison with the heat-transfer coefficient, and they neglected temperature variations in the solid. Thus, they were able to obtain both steady-state and transient solutions for the average temperature of the material.

Recently, Zinn and Mader (Ref. 8) attacked the full partial differential equation (Eq. 1) by numerical means, using high-speed computing equipment. They worked with the slab, the cylinder,

and the sphere with the surfaces held at sufficiently high constant temperatures that a steady state was not possible, and they determined the transient temperature distributions and the time that would elapse before the material exploded.

Using the work of the authors cited, it is now possible to determine the steady-state temperature distributions and, more important, the maximum conditions for which a steady-state solution is possible for several combinations of geometry and boundary conditions. In some circumstances it becomes necessary to exceed the maximum conditions for which a steady-state solution is possible, and, thus, if these conditions were exceeded for a sufficient length of time, the material would explode. It is now possible, for constant-temperature surfaces on the slab, the cylinder, and the sphere (corresponding to very large heat-transfer coefficients), to determine how long the material will take to explode. This information is important to engineers who process explosives or design weapons.

### DESCRIPTION OF THE PROBLEM

The differential equation for the steady state, Eq. 2, can be put into dimensionless form as

$$\frac{d^2\theta}{d\omega^2} + \left(\frac{k}{\omega}\right)\left(\frac{d\theta}{d\omega}\right) = \delta \exp \theta \quad (3)$$

in which

$$\delta = \frac{\rho Q Z E a^2}{\lambda R T_0^2} \exp(-E/RT_0) \quad (4)$$

$$\theta = \frac{E}{RT_0^2} (T - T_0) \quad (5)$$

$$\omega = r/a \quad (6)$$

and  $k = 0, 1$ , and  $2$ , respectively, for the slab, the cylinder, and the sphere. Boundary conditions of the type

$$h(T_s - T_0) + \lambda(dT/dr)_s = 0 \quad (7)$$

become

$$(ha/\lambda)\theta_s + (d\theta/d\omega)_s = 0 \quad (8)$$

If the dimensionless ratio  $ha/\lambda$  is zero, the surface is adiabatic; if the ratio is infinite, the surface assumes the temperature of the surroundings,  $T_0$ . For intermediate ratios, the surface temperature is somewhat higher than that of the surroundings.

The critical temperature of an object is defined as the maximum temperature of the surroundings imposed on the object in some specified fashion for which a steady state is possible. It follows, therefore, that, if the surroundings are held at a temperature greater than the critical temperature for the specified situation, the object will self-heat until it ignites or explodes.

The maximum or critical values of the parameter  $\delta$  have been given by several authors (Ref. 1-6) for various geometries and boundary conditions. Values for the slab, the solid cylinder, and the sphere have been given by Frank-Kamenetski and Chambré. These correspond to boundary conditions with infinite heat-transfer coefficients and represent values of  $\delta$  of 0.88, 2.00, and 3.32, respectively.

Table 1 shows values of  $\delta$  for hollow cylinders as functions of the ratio of inner- to outer-radius. Two sets of boundary conditions are included. The first is for the same surface tempera-



TABLE 1. SHAPE FACTORS FOR THE HOLLOW CYLINDER

Radius ratio	Shape factor, $\delta$	
	Same temperature inside and outside	Adiabatic inside, constant temperature outside
0.025	3.008	2.003
0.05	3.320	2.020
0.10	3.892	2.077
0.15	4.492	2.172
0.20	5.171	2.306
0.25	5.966	2.483
0.30	6.921	2.713
0.35	8.091	3.004
0.40	9.556	3.384
0.45	11.43	3.878
0.50	13.88	4.530
0.55	17.19	5.413
0.60	21.81	6.646
0.65	28.55	8.434
0.70	38.91	11.17
0.75	56.10	15.69
0.80	87.73	23.92
0.85	156.1	41.57
0.90	351.3	91.50
0.95	1405	358.4
1.00	$\infty$	$\infty$

ture inside and out; the second is adiabatic inside and constant surface temperature outside. Thus, the first set of boundary conditions corresponds to infinite heat-transfer coefficients and the same temperature of surroundings inside and out. The values of  $\delta$  are those given by Enig in Ref. 3. The second set of boundary conditions corresponds to an infinite heat-transfer coefficient on the outside and a zero heat-transfer coefficient on the inside. The values of  $\delta$  for radius ratios less than 0.35 were calculated using equations given by Conrad and Longwell in Ref. 4, and those for the remaining ratios were derived from the results of Enig as described previously.

Table 2 gives values of  $\delta$  for finite heat-transfer coefficients for the slab, cylinder, and sphere. These values were read from graphs presented by Thomas in Ref. 6 and are given as functions of the dimensionless ratio  $ha/\lambda$ .

Knowing  $\delta$ , the critical temperature may be calculated from Eq. 4, which can be arranged to give

$$T_m = \frac{E}{2.303R \log (\rho a^2 QZE / \lambda R T_m^2 \delta)} \quad (9)$$

The temperatures are absolute temperatures expressed in degrees Kelvin, and the activation energy,  $E$ , is in cal/mole; not, as it is usually quoted, in kcal/mole. The units and definitions of the various quantities are listed in the nomenclature.

Zinn and Mader (Ref. 8) presented a graph showing the dimensionless parameter  $F = \lambda t_e / \rho c a^2$  as a function of  $E(1/T_m - 1/T_1)$  for the slab, the cylinder, and the sphere. The boundary conditions are that the surface is held at the temperature  $T_1$ , which is above the critical temperature,

TABLE 2. SHAPE FACTORS WITH FINITE  
HEAT-TRANSFER COEFFICIENTS

Dimensionless ratio, $ha/\lambda$	Shape factor, $\delta$		
	Slab	Cylinder	Sphere
0	0	0	0
1	0.26	0.55	0.87
2	0.42	0.91	1.47
3	0.51	1.13	1.86
4	0.57	1.28	2.13
5	0.61	1.39	2.31
6	0.63	1.47	2.43
8	0.68	1.58	2.59
10	0.71	1.67	2.74
12	0.74	1.73	2.83
14	0.76	1.77	2.91
$\infty$	0.88	2.00	3.32

and thus correspond to an infinite heat-transfer coefficient to surroundings at  $T_1$ . In order to calculate a time-to-explosion,  $t_e$ , the critical temperature is first calculated from Eq. 9, then the quantity  $E(1/T_m - 1/T_1)$  is calculated, and  $F$  read from the graph. Finally,  $t_e$  is calculated from the value of  $F$ .

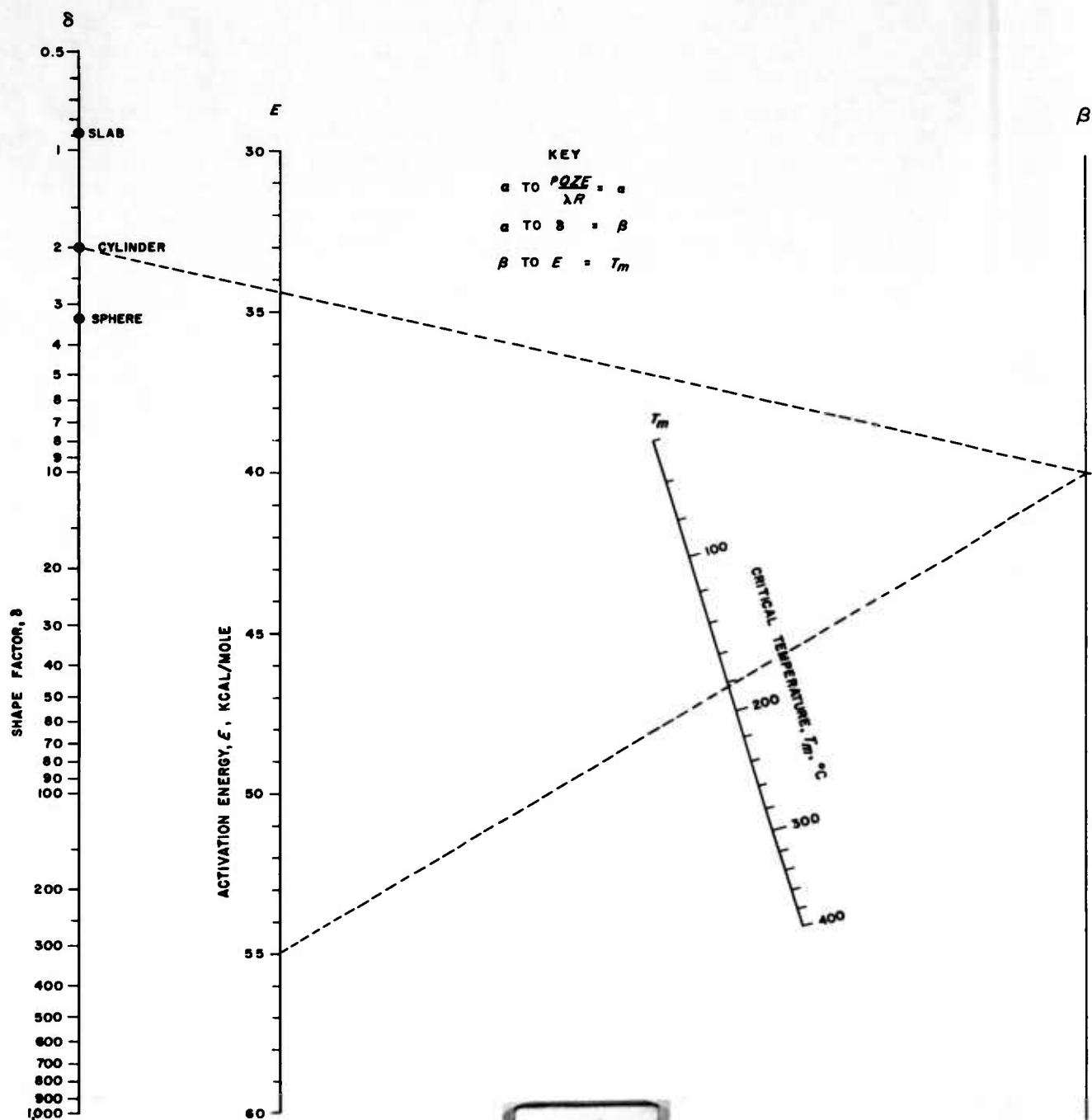
### USE OF NOMOGRAPHS

The calculations of the critical temperature and of the time-to-explosion can be done easily by the use of nomographs that have been constructed. These nomographs have the usual advantages, such as rapidity of use, reduction of the likelihood of making errors, and the presentation of results in desired units and can be used by persons who are not thoroughly conversant with the calculations represented. The construction of these nomographs is described in the Appendix; their use is described below.

### CRITICAL TEMPERATURE

The critical temperature of an object is the maximum temperature of the surroundings imposed on the object in some specified fashion for which a steady state is possible. In order to calculate the critical temperature using Nomograph 1, seen in Fig. 1, four quantities are needed:

1.  $a$ , the half-thickness of a slab, or the exterior radius of a cylinder or sphere, expressed in cm.
2. The quantity  $\rho QZE/\lambda R$ , expressed in  $^{\circ}\text{K}^2/\text{cm}^2$ . Note that  $E$  must be expressed in cal/mole in calculating this quantity. The quantity  $QZ$  is in cal/g-sec.
3.  $E$ , the activation energy, expressed in kcal/mole.
4. The critical value of the shape factor  $\delta$  for the specific geometry and boundary conditions. Values of  $\delta$  can be obtained as follows:
  - a. Slab, solid cylinder, or sphere, with infinite heat-transfer coefficient (constant-temperature surface): use points labeled "slab," "cylinder," or "sphere" on the  $\delta$  axis of Nomograph 1.
  - b. Hollow cylinder, infinite heat-transfer coefficients inside and outside, same temperature inside and outside: use Table 1, column headed "Same temperature inside and outside" for proper ratio of inside-to-outside radii.



1

FIG. 1. Nomograph 1.

KEY  
 $a$  TO  $\frac{PQZE}{\lambda R} = a$   
 $a$  TO  $\beta = \beta$   
 $\beta$  TO  $E = T_m$

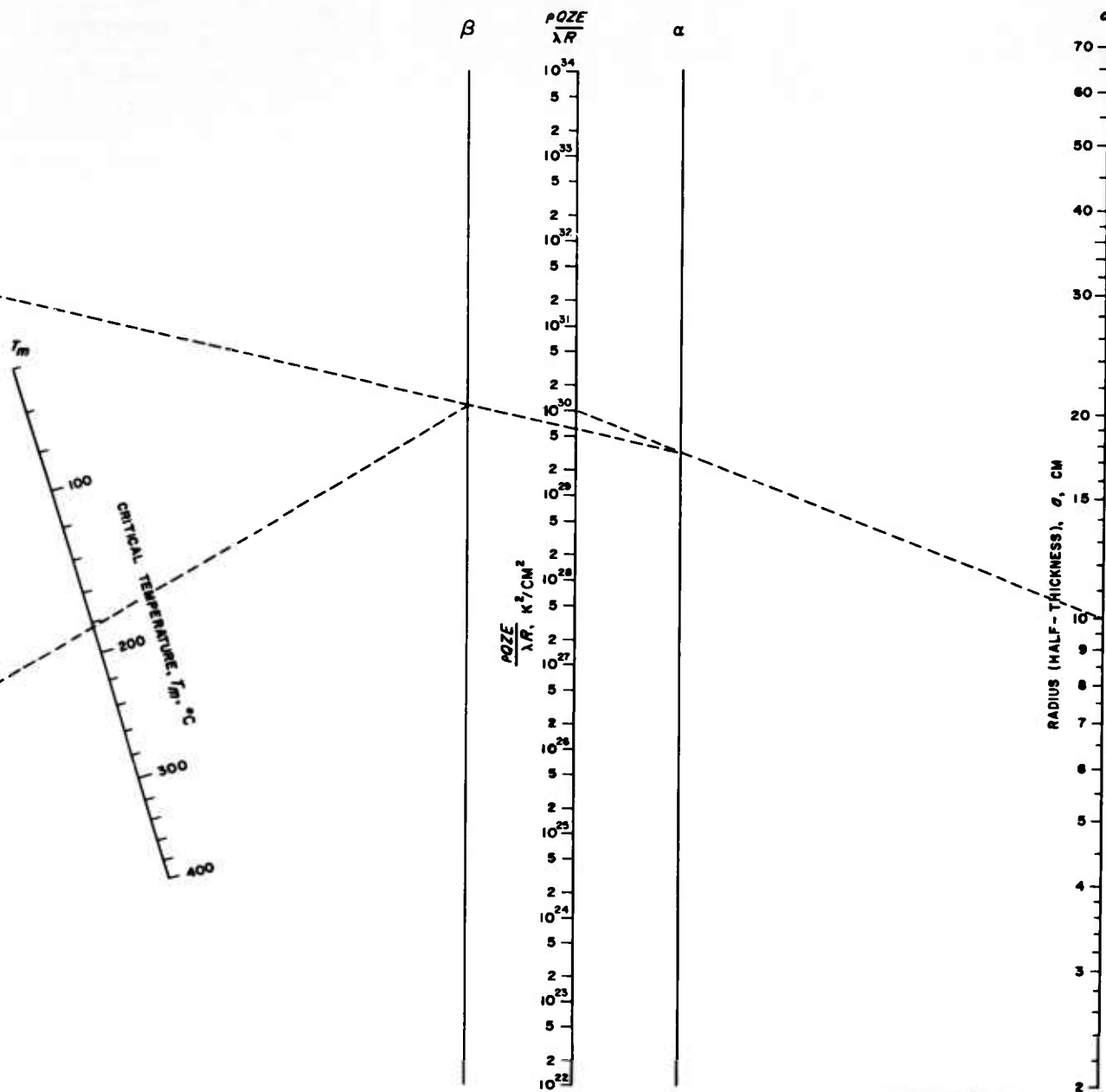


FIG. 1. Nomograph 1.

- c. Hollow cylinder, infinite heat-transfer coefficient outside, zero heat-transfer coefficient inside: use Table 1, column headed "Adiabatic inside, constant temperature outside" for proper ratio of inside-to-outside radii.
- d. Slab, solid cylinder, or sphere, with finite heat-transfer coefficient: calculate  $ha/\lambda$ , take value of  $\delta$  from Table 2.

The use of Nomograph 1 is shown by the key. A straight line drawn between  $a$  and  $\rho QZE/\lambda R$  intersects the  $\alpha$  axis at a point  $\alpha$ , a straight line between the point  $\alpha$  and the value of  $\delta$  intersects the  $\beta$  axis at a point  $\beta$ , and a straight line between the point  $\beta$  and the value of  $E$  intersects the  $T_m$  axis at a point that is read as the critical temperature,  $T_m$ . On the nomographs, the temperatures are expressed in degrees centigrade in order to facilitate calculations.

This will be demonstrated by four examples, one for each of the four general types of situations presented above for shape factors  $\delta$ .

**Example 1.** A solid cylinder 20 cm in diameter, composed of material having  $E = 55$  kcal/mole and  $\rho QZE/\lambda R = 1.0 \times 10^{30}$  °K<sup>2</sup>/cm<sup>2</sup>, has its exterior surface held at constant temperature. Presume the length-to-diameter ratio is large, so the end effects are negligible, and the point labeled "cylinder" on the  $\delta$  axis, corresponding to  $\delta = 2.00$ , is appropriate. Using  $a = 10$  cm and the other data as given, Nomograph 1 gives a critical temperature,  $T_m$ , of 182°C. The construction is shown dotted on the nomograph. A numerical calculation using Eq. 9 gives 455.6°K (182.4°C).

**Example 2.** A hollow cylinder 6.0 inches in outside diameter and 3.9 inches in inside diameter is held at the same constant temperature on both surfaces.  $E = 44$  kcal/mole and  $\rho QZE/\lambda R = 5 \times 10^{27}$  °K<sup>2</sup>/cm<sup>2</sup>. Presume the length-to-diameter ratio is large, so Table 1 can be used. The radius ratio is  $3.9/6.0 = 0.65$  and, from Table 1,  $\delta = 28.55$ .  $a = 6.0 \times 2.54/2 = 7.62$  cm. The critical temperature is read from Nomograph 1 as 149°C. As a check, the numerical calculation using Eq. 9 gives 422.5°K (149.3°C).

**Example 3.** The hollow cylinder of Example 2 is held at a constant temperature on the outside, but there is no heat transfer on the inside. Table 1 is used with the radius ratio of 0.65, giving  $\delta = 8.434$ .  $a = 7.62$  cm,  $E = 44$  kcal/mole, and  $\rho QZE/\lambda R = 5 \times 10^{27}$  °K<sup>2</sup>/cm<sup>2</sup>. The nomograph gives 139°C as the critical temperature. As a check, the numerical calculation gives 412.6°K (139.4°C).

**Example 4.** A sphere 20 cm in diameter is suspended in an air stream, and the heat-transfer coefficient is estimated at 2.0 Btu/ft<sup>2</sup>-hr-°F. The thermal conductivity of the material is 0.2 Btu/hr-ft-°F.  $E = 55$  kcal/mole, and  $\rho QZE/\lambda R = 1.0 \times 10^{30}$  °K<sup>2</sup>/cm<sup>2</sup>.  $a$  is 10 cm. The parameter  $ha/\lambda$  must be calculated, watching units so that the result is dimensionless. In this case,  $h$  must be converted to cal/cm<sup>2</sup>-sec-°C and  $k$  to cal/cm-sec-°C, or the radius converted to feet. Doing the latter,  $a = 10/(12 \times 2.54) = 0.328$  foot and  $ha/\lambda = 2.0(0.328)/0.20 = 3.28$ . Using Table 2,  $\delta$  is interpolated as 1.94. The nomograph gives 182°C. The numerical calculation gives 455.3°K (182.1°C).

## TIME-TO-EXPLOSION

The time-to-explosion,  $t_e$ , can currently *only* be calculated for the slab, the solid cylinder, and the sphere and with the outside surfaces held at a constant temperature corresponding to an infinite heat-transfer coefficient. This constant temperature, designated as  $T_1$ , is larger than the critical temperature for the infinite heat-transfer coefficient. The time-to-explosion,  $t_e$ , is calculated using Nomographs 2 and 3 (Fig. 2 and 3), and the following data are required in addition to those required to calculate the critical temperature using Nomograph 1.

1.  $T_1$ , the constant-temperature surface, °C.
2. The quantity  $\rho c/\lambda$ , sec/cm<sup>2</sup>.

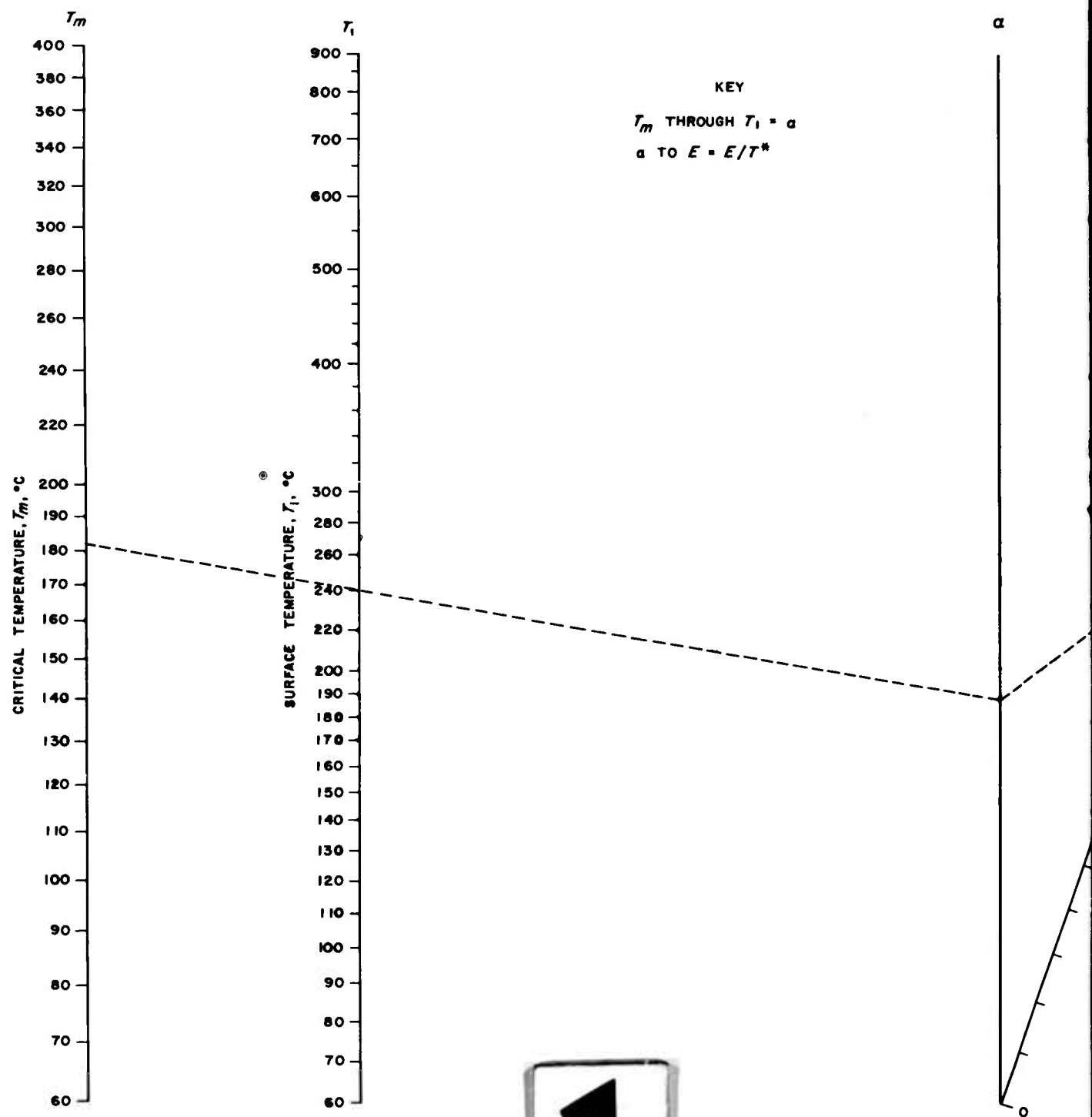


FIG. 2. Nomograph 2.

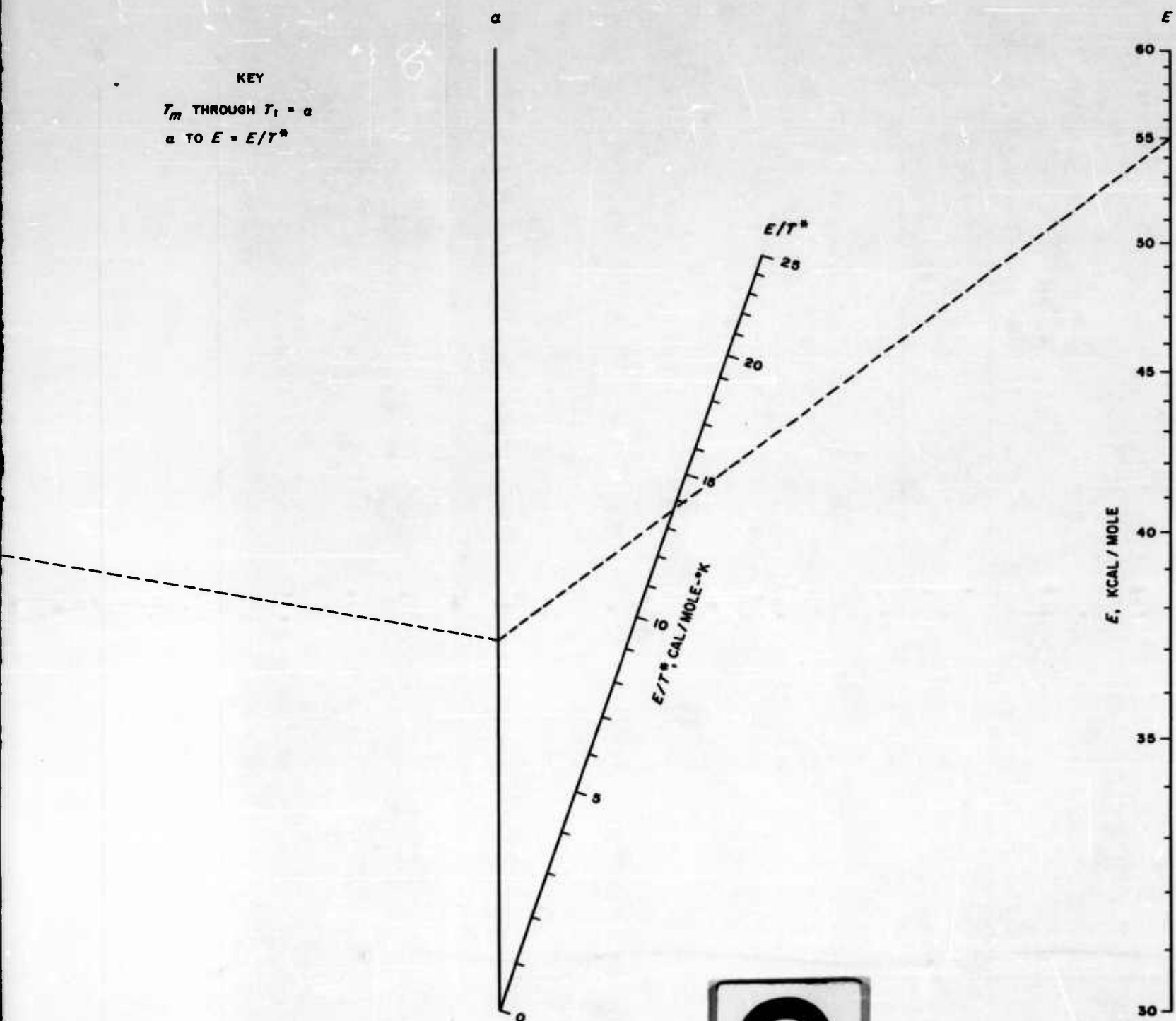


FIG. 2. Nomograph 2.

2

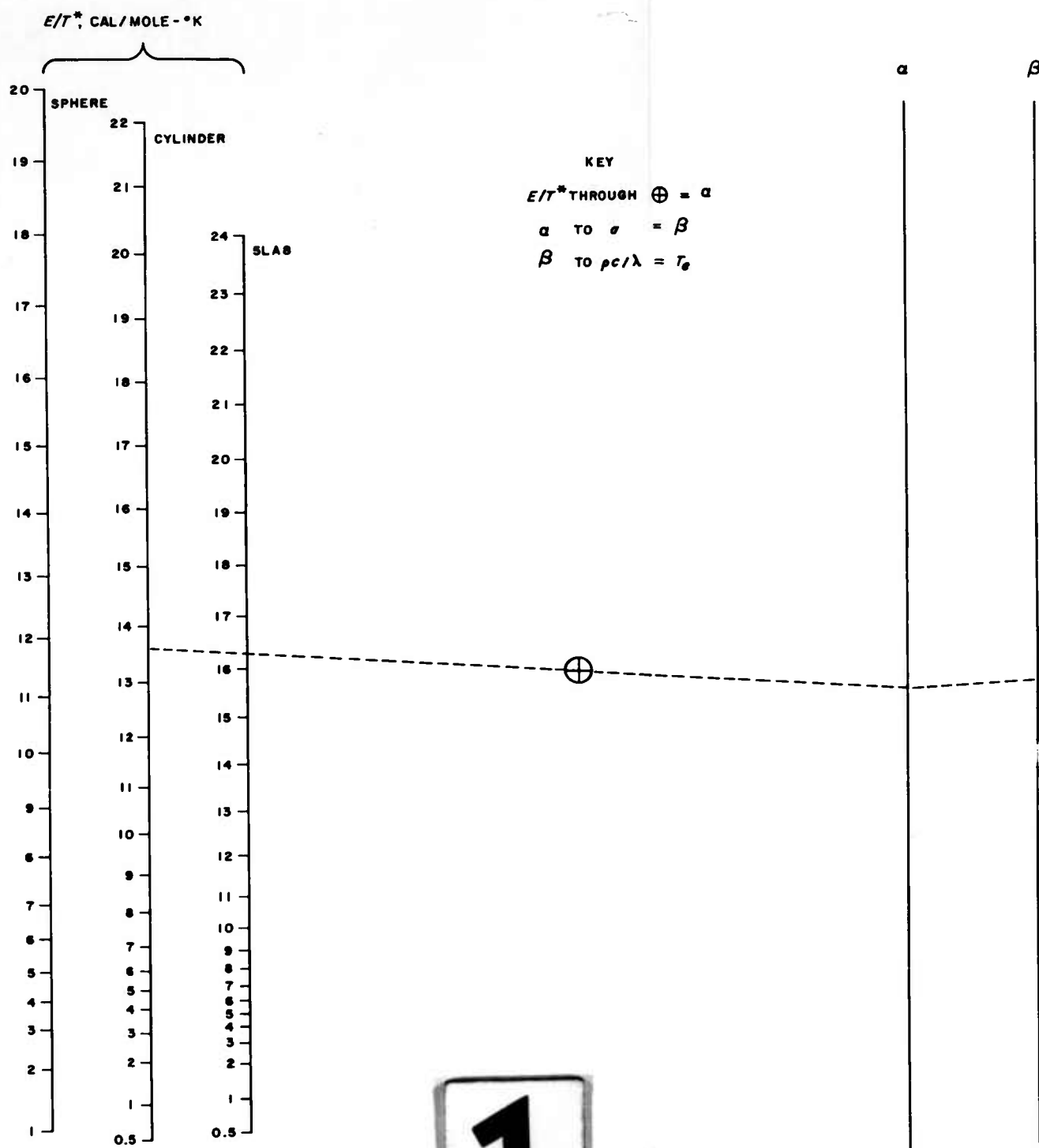


FIG. 3. Nomograph 3.



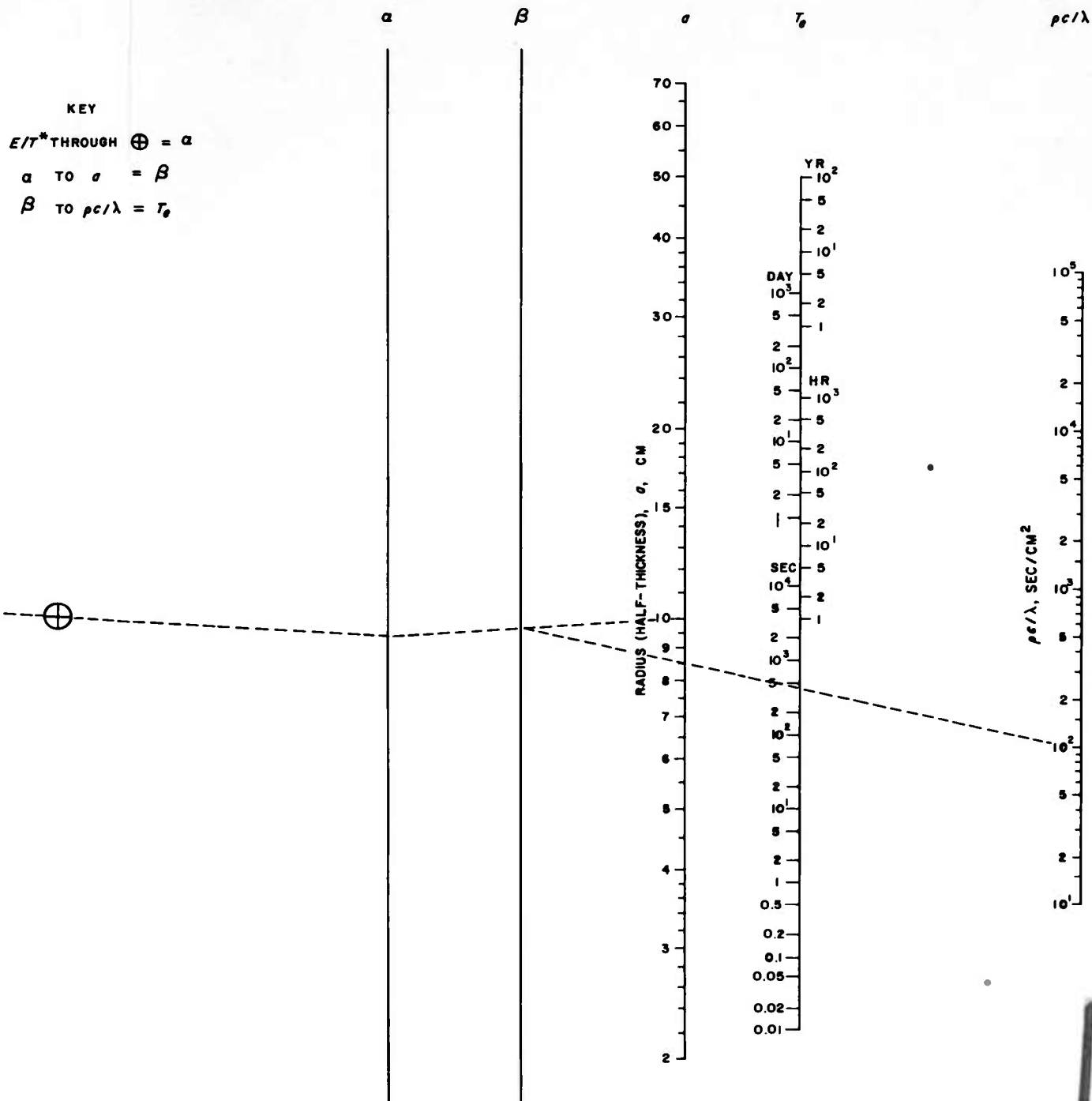


FIG. 3. Nomograph 3.

The critical temperature,  $T_m$ , is calculated for the constant-temperature surface as described above and shown in Example 1. Nomograph 2 is used as shown by the key. It is entered with  $T_m$  and  $T_1$ , which are connected by a straight line intersecting the  $\alpha$  axis at a point  $\alpha$ . The point  $\alpha$  is connected with  $E$  by a straight line that intersects the  $E/T^*$  axis at a point where the value is read as  $E/T^*$ . This value is taken to Nomograph 3, and the corresponding point on the appropriate  $E/T^*$  axis (sphere, cylinder, or slab) is connected to the  $\alpha$  axis by a straight line through the point marked  $\oplus$ . The intersection on the  $\alpha$  axis is connected with the value of  $a$  on the  $a$  axis to give an intersection on the  $\beta$  axis, and the latter is connected with the value of  $\rho c/\lambda$  by a straight line that intersects the  $t_e$  axis at the time-to-explosion.

This calculation is illustrated by an example.

*Example 5.* A long, solid cylinder 10 cm in radius, composed of materials having  $E = 55$  kcal/mole,  $\rho QZE/\lambda R = 1.0 \times 10^{30} \text{ } ^\circ\text{K}^2/\text{cm}^2$ , and  $\rho c/\lambda = 500 \text{ sec/cm}^2$ , has its exterior surface held at  $240^\circ\text{C}$ . The critical temperature for the constant-temperature surface was found in Example 1 to be  $182^\circ\text{C}$ . Using  $T_m = 182^\circ\text{C}$  and  $T_1 = 240^\circ\text{C}$ , the value of  $E/T^*$  is read from Nomograph 2 as  $13.7 \text{ cal/mole-}^\circ\text{K}$ . This value is used on the cylinder  $E/T^*$  axis of Nomograph 3 and, using the given values of  $a$  and  $\rho c/\lambda$ , the time-to-explosion is read as 2,500 seconds. As a check by numerical calculation,  $T_m$  was found to be  $182.4^\circ\text{C}$  in Example 1. Using this value and the given values of  $T_1$  and  $E$ ,  $E/T^*$  is calculated as  $13.55 \text{ cal/mole-}^\circ\text{K}$ . Again using this calculated value and the given values of  $a$  and  $\rho c/\lambda$ ,  $t_e$  is found to be 2,450 seconds.

## COMMENTS AND CAUTIONS

The nomographs accompanying this report allow fairly accurate solutions of certain mathematical problems, and, if physical problems are well described by the mathematics involved, the solutions of the physical problems can be equally well determined. As a matter of fact, the physical problems are not always as simple as the mathematical problem described by Eq. 1 and the associated initial and boundary conditions.

The major trouble is that the reaction rate may not be well described by an expression of the type  $QZ \exp(-E/RT)$ , in which all parameters except the temperature are constants. Decomposition reactions are sometimes autocatalytic or catalyzed by small amounts of impurities, so that the decomposition rate is a function of duration or extent of decomposition, and, if this is true to a significant extent, the analysis described herein is not suitable. If an autocatalytic reaction, such as the decomposition of nitrocellulose, is controlled by the use of stabilizers, the relations used can only be valid as long as the stabilizer remains and is effective.

Appropriate values of the physical constants must be known. Determinations of thermal conductivity, specific heat, and density can be relatively precise, but the measurement of the reaction-rate parameters  $QZ$  and  $E$  is difficult, and the accuracy of such parameters is generally much poorer. Generally, the accuracies of these two parameters are the limiting factors on the accuracy of determination of critical temperatures or times-to-explosion, even though the decomposition reactions do appear to be well behaved.

No phase changes have been considered in this treatment. If phase changes occur, the critical temperature should not be affected appreciably, but the time-to-explosion will probably be somewhat greater than calculated.

As a result, the values of critical temperature and time-to-explosion determined should be considered as only approximate. They should be used with margins of safety dictated by engineering judgments that are strongly influenced by the magnitude of the cost of being wrong.

# Appendix DETAILS OF CONSTRUCTION OF NOMOGRAPHS

## NOMOGRAPH 1

This nomograph solves the equation for the critical temperature.

$$T_m = \frac{E}{2.303R \log(\rho a^2 QZE / \lambda R T_m^2 \delta)} \quad (10)$$

Rearranging Eq. 10 gives

$$2T_m \log T_m = T_m \log \left[ \left( \frac{\rho QZE}{\lambda R} \right) \left( \frac{a^2}{\delta} \right) \right] - \frac{E}{2.303R} \quad (11)$$

which can be put in the form of Type C of Davis (Ref. 9) as

$$f(x) = \psi(x) \cdot F(y) + \phi(z) \quad (12)$$

with

$$\begin{aligned} f(x) &= 2T_m \log T_m & \psi(x) &= T_m \\ F(y) &= \log \left[ \left( \frac{\rho QZE}{\lambda R} \right) \left( \frac{a^2}{\delta} \right) \right] & \phi(z) &= \frac{E}{2.303R} \end{aligned} \quad (13)$$

The value of  $F(y)$  is calculated using logarithmic charts described by Davis as Type B, which are really addition charts (Davis Type A) in terms of logarithms. The modulus of a particular scale is defined as the distance along the scale for one unit of the linearly plotted variable. For example, in Nomograph 1, the right-hand scale, labeled  $a$ , is actually a linear scale in terms of  $\log a^2$  and the modulus of this scale,  $M_a$ , was taken as 10 cm per unit change in  $\log a^2$ .

Referring to Fig. 4, which shows an addition chart solving the equation,

$$f(x) = F(y) + \phi(z) \quad (14)$$

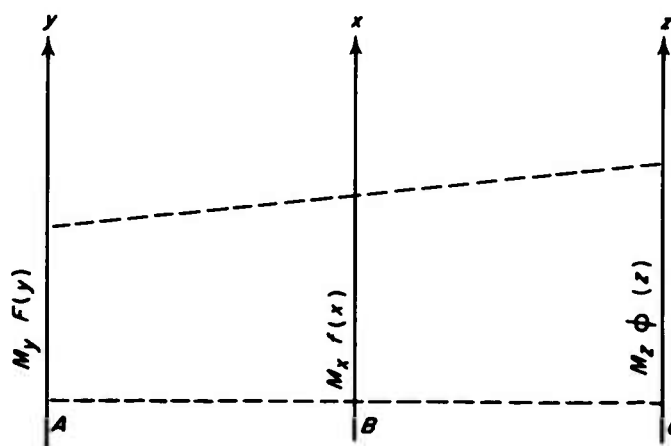


FIG. 4. Addition Chart.

it is necessary that

$$M_x = \frac{M_y M_z}{M_y + M_z} \quad (15)$$

and that

$$\frac{AB}{BC} = \frac{M_y}{M_z} \quad (16)$$

Thus, the selection of two moduli automatically establishes the modulus and relative position of the third scale.

Nomograph 1 proceeds as follows:

First,  $\alpha$  is calculated as

$$\alpha = \log \left( \frac{\rho Q Z E}{\lambda R} \right) + \log a^2 \quad (17)$$

with  $M_a = 10$  cm and the modulus of  $(\rho Q Z E)/(\lambda R) = 2.5$  cm, giving  $M_\alpha = 2.0$  cm and scale spacing from  $\alpha$  in the ratio of 4 to 1, which was used as 12 cm and 3 cm.

Next,  $\beta$  was calculated as

$$\beta = \alpha + \log (1/\delta) = \alpha - \log \delta \quad (18)$$

with  $M_\alpha = 2.0$ ,  $M_\delta = 10.0$ , giving  $M_\beta = 1.667$  and scale spacing from  $\beta$  in the ratio of 1 to 5, which was used as 6 cm and 30 cm. Thus,

$$\beta = \log \left[ \left( \frac{\rho Q Z E}{\lambda R} \right) \left( \frac{a^2}{\delta} \right) \right] = F(y) \quad (19)$$

The recurrent-variable equation shown above as Eq. 11 and 12 may now be solved. The construction is shown in Fig. 5. The point  $F$ , which is located on the line connecting the given values of  $\phi(z)$  and  $F(y)$ , is the location for the desired value of  $f(x)$ . It is located in accordance with the relations

$$\frac{CE}{CA} = \left[ \frac{M_z}{M_z \psi(x) + M_y} \right] \psi(x) \quad (20)$$

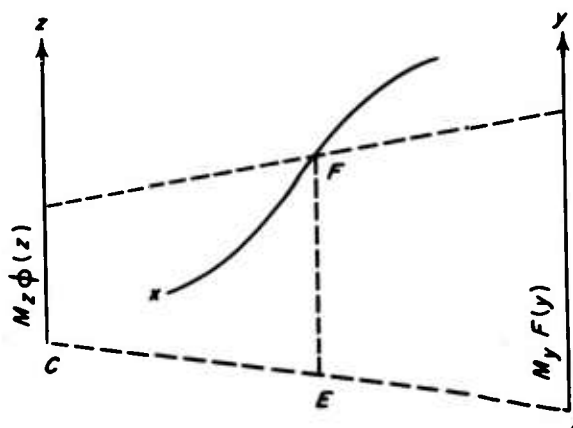


FIG. 5. Recurrent-Variable Chart.

$$EF = \left[ \frac{M_y M_z}{M_z \psi(x) + M_y} \right] f(x) \quad (21)$$

Points  $C$  and  $A$  are located where  $\phi(z)$  and  $F(y)$  are respectively equal to zero, and, thus, the line  $CEA$  is between the zeros of the two scales.

For Nomograph 1,  $M_y = M_\beta = 1.667$ , and  $M_z = 4.575 \times 10^{-3}$ , where  $M_z$  is in terms of  $E/2.303R$ . The scale on Nomograph 1 is marked in terms of  $E$ , using the modulus of  $1.00 \times 10^{-3}$  cm/kcal-mole, which is consistent with  $M_z$ . The spacing between the  $E$  scale and the  $\beta$  scale was made 24 cm, and, taking the origin of Cartesian coordinates  $(x, y)$  at the 60 kcal/mole point on the  $E$  scale and with the other scales as shown on Nomograph 1, the points for the critical temperature,  $T_m$  (expressed in degrees Kelvin), are located at  $(x, y)$  where

$$x = \frac{24T_m}{T_m + 364.4} \quad (22)$$

and

$$y = 60 - 3.8611x + 0.13888x \log T_m \quad (23)$$

The  $T_m$  scale was graduated in terms of degrees Centigrade and the  $E$  scale in terms of kcal/mole, although these variables must be expressed in terms of degrees Kelvin and cal/mole, respectively, in the equations.

## NOMOGRAPH 2

This nomograph calculates  $E/T^*$  from  $E$ , the critical temperature  $T_m$  obtained from Nomograph 1, and the constant-temperature surface  $T_1$ , according to the equation

$$E/T^* = E(1/T_m - 1/T_1) \quad (24)$$

First, an addition chart (Davis Type A) is used to calculate

$$\alpha = 1/T^* = (1/T_m - 1/T_1) \quad (25)$$

which is actually done in the form

$$1/T_1 = 1/T_m - \alpha \quad (26)$$

Moduli satisfying Eq. 15 were selected as  $M_{T_m} = 2.0 \times 10^4$  cm-°K,  $M_\alpha = 4.667 \times 10^4$  cm-°K, and  $M_{T_1} = 1.4 \times 10^4$  cm-°K, and the distances between scales  $T_m$  to  $T_1$  and  $T_1$  to  $\alpha$  as 7.5 cm and 17.5 cm, respectively. The scales  $T_m$  and  $T_1$  were calculated as inverse absolute temperatures and graduated in degrees Centigrade. The scale,  $\alpha$ , calculated as inverse absolute temperature, increases in the direction opposite to the other two scales.

Next,  $E/T^*$  is calculated from

$$E/T^* = (\alpha)(E) \quad (27)$$

The scale for  $\alpha$  is linear, not logarithmic, so a nonlogarithmic multiplication chart of Type D as described by Davis was employed. This type is constructed as shown in Fig. 6 for the equation

$$f(x) = F(y)/\phi(z) \quad (28)$$

The scales for  $F(y)$  and  $\phi(z)$  are laid out in opposite directions using the moduli  $M_y$  and  $M_z$ , starting with zeros at points  $A$  and  $C$ , respectively. The  $x$  axis connects points  $A$  and  $C$ . A point,  $H$ , is selected on the  $z$  axis with  $CH = h$ , and a temporary auxiliary scale with modulus  $M = hM_y/M_z$  is constructed on the  $y$  axis starting at  $A$ . The  $x$  scale on the  $x$  axis is constructed by projecting the auxiliary scale by means of straight lines through the point  $H$ .

A disadvantage of this type of nomograph is that the scale for  $f(x)$  is likely to be quite compressed. Several permutations of Eq. 27 are possible, and it was found that the largest scales

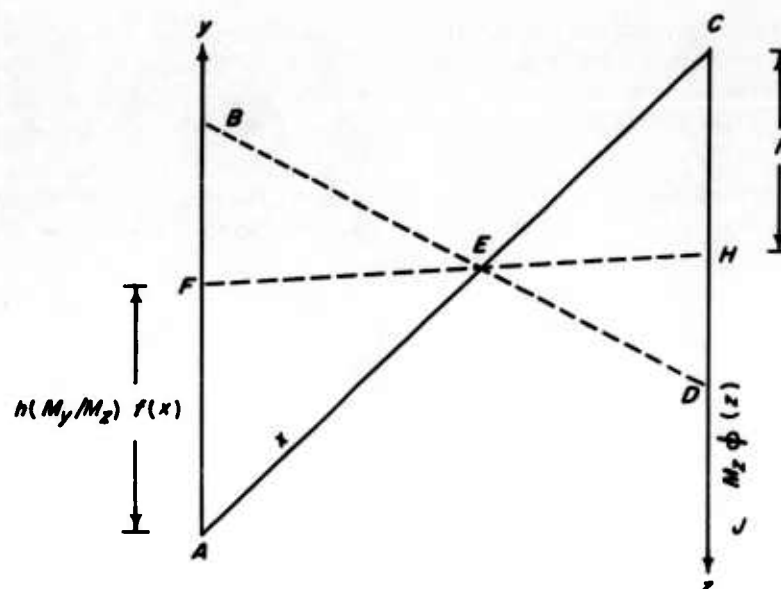


FIG. 6. Nonlogarithmic Multiplication Chart.

could be obtained by using  $f(x) = E/T^*$ ,  $F(y) = \alpha$ , and  $\phi(z) = 1/E$ . Rather than actually constructing the auxiliary scale and doing the construction by projection, an algebraic expression for the location of points on the  $x$  scale was derived. Taking the origin at point  $A$  of Fig. 3, letting  $y$  now be the vertical Cartesian coordinate of the point  $f(x)$  on the  $x$  axis, and with the elevation of point  $C$  above the horizontal axis being  $CJ$ , the expression is

$$\frac{y}{CJ} = \frac{M_y F(y)}{M_x \phi(z) + M_y F(y)} = \frac{f(x)}{f(x) + M_x/M_y} \quad (29)$$

Taking  $M_y = M_\alpha = 4.667 \times 10^4$  cm-°K, and  $M_x = 1.8 \times 10^6$  cm-kcal/mole, and  $CJ = 60$  cm, Eq. 29 becomes

$$y = \frac{60(E/T^*)}{(E/T^*) + 38.57} \quad (30)$$

which was used to compute the  $E/T^*$  scale of Nomograph 2. The  $E$  scale was calculated in terms of  $1/E$  in mole/cal, but graduated as  $E$  in kcal/mole.

### NOMOGRAPH 3

Zinn and Mader presented a graph of the quantity  $F = \lambda T_e / \rho c a^2$  as a function of the quantity  $E/T^*$ , showing curves for the slab, the cylinder, and the sphere. Nomograph 3 is entered with  $E/T^*$  and determines the value of  $\log F$  as  $\alpha$ , then calculates  $t_e$  from the equation

$$t_e = F(a^2)(\rho c / \lambda) \quad (31)$$

The first operation amounts essentially to reading the graph to determine  $F$  for the appropriate geometry and given value of  $E/T^*$ .

The  $\alpha$  scale was assigned a modulus ( $M_\alpha$ ) of 8.0 cm. A swing point was located midway between the slab axis and the  $\alpha$  axis, 10 cm from each. The slab axis thus has a modulus of 8.0 cm.

The cylinder axis was located 3 cm to the left of the slab axis and has a modulus of  $8.0(10 + 3)/10 = 10.4$ ; the sphere axis, located 3 cm to the left of the cylinder axis, has a modulus of  $8.0(10 + 6)/10 = 12.8$ . In order to make  $\alpha$  increase upward, the scales for the three shape axes increase downward in terms of  $\alpha$ ; however, they are graduated in terms of  $E/T^*$ , which increases upward.

Measuring  $y$  upward from a horizontal base line intersecting the  $\alpha$  axis at  $-3.00$ , the swing point was located at  $y = 14.0$  cm, and the scales on the three shape axes then were graduated in terms of  $E/T^*$  at the locations

$$\begin{aligned} y &= 28.0 - 8.0 (\log F + 3.0) \text{ slab} \\ y &= 32.2 - 10.4 (\log F + 3.0) \text{ cylinder} \\ y &= 36.4 - 12.8 (\log F + 3.0) \text{ sphere} \end{aligned} \quad (32)$$

in which the values of  $\log F$  were read from the appropriate curve on a large scale graph supplied by Mader.<sup>1</sup>

The next operation is to calculate  $\beta$  from

$$\beta = \log Fa^2 = \alpha + \log a^2 \quad (33)$$

This is done by addition. The  $a$  scale has a modulus of 10.0 cm in terms of  $\log a^2$ , and, as  $M_\alpha = 8.0$  cm,  $M_\beta$  is 4.444 cm, and the spacings of the  $\alpha$  and  $a$  axes from the  $\beta$  axis are 4 and 5 cm, respectively. The  $a$  scale was graduated in terms of  $a$  at the positions given by the equation

$$y = 20 \log a - 6 \quad (34)$$

The  $\alpha$  scale and the  $\beta$  scale are not graduated, as these intermediate results need not be read.

The final operation is to calculate  $t_e$  from

$$\log t_e = \beta + \log (\rho c / \lambda) \quad (35)$$

which is also done by addition. A modulus of the  $\log (\rho c / \lambda)$  scale was selected as 5.0 cm, and, as  $M_\beta = 4.444$  cm,  $M_t = 2.353$  cm in terms of  $\log t_e$ . The  $\beta$  and  $(\rho c / \lambda)$  scales are, respectively, 8 and 9 cm from the  $t_e$  scale. The  $\log (\rho c / \lambda)$  scale was graduated in terms of  $(\rho c / \lambda)$  at the position

$$y = 5 \log (\rho c / \lambda) \quad (36)$$

The  $\log t_e$  scale is appropriately graduated in terms of  $t_e$  expressed in seconds, and the corresponding positions are given by

$$y = 5.647 + 2.353 \log t_e \quad (t_e, \text{ seconds}) \quad (37)$$

However, it was believed appropriate to convert the large values of  $t_e$  to larger units of time, so Eq. 37 was used for a range of  $10^{-2}$  to  $10^4$  seconds, and the alternate equations following were used for a larger  $t_e$ .

$$y = 11.015 + 2.353 \log t_e \quad (t_e, \text{ hours}) \quad (38)$$

$$y = 14.263 + 2.353 \log t_e \quad (t_e, \text{ days}) \quad (39)$$

$$y = 20.292 + 2.353 \log t_e \quad (t_e, \text{ years}) \quad (40)$$

<sup>1</sup> Private communication to D. Lind from Charles L. Mader, September 1960.

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